

NMR Study of 3,5-Dichloropyridine in the Nematic Phase of the Liquid Crystal

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The importance of NMR studies on oriented molecules dissolved in the nematic phase of liquid crystals is well recognized¹. The aim of this note is to report such a study of 3,5-dichloropyridine in the nematic phase of N-(p-Methoxy-benzyliden)-p-n-butylanilin (MBBA). The observed spectrum is that of an AB₂ symmetry with nine detected lines (Fig. 1). The analysis¹ of this spectrum is straightforward and the values for the direct (*D*) coupling constants, the indirect (*J*) coupling constants and the elements of the orientation matrix *S* are:

$$\begin{aligned} D_{AB} &= -51 \text{ Hz}, & S_{11} &= 0.003, \\ D_{BB} &= -241 \text{ Hz}, & S_{22} &= 0.139, \\ J_{AB} &= \pm 2 \text{ Hz}, \end{aligned}$$

J was supposed to have the same value as in the isotropic phase and elements of the *S* matrix were obtained by using the geometry of pyridine². The values of *D* suggest that the molecule is preferentially oriented with the axes B—B along the magnetic field. The anisotropies of the chemical shifts are $\sigma_a = 0.46$ ppm for protons A and $\sigma_a = 0.06$ ppm for protons B. These shifts are towards higher fields and support the mentioned conclusion about the orientation of the molecule. We could not explain in a simple manner why the chemical shifts are so different for A and B protons.

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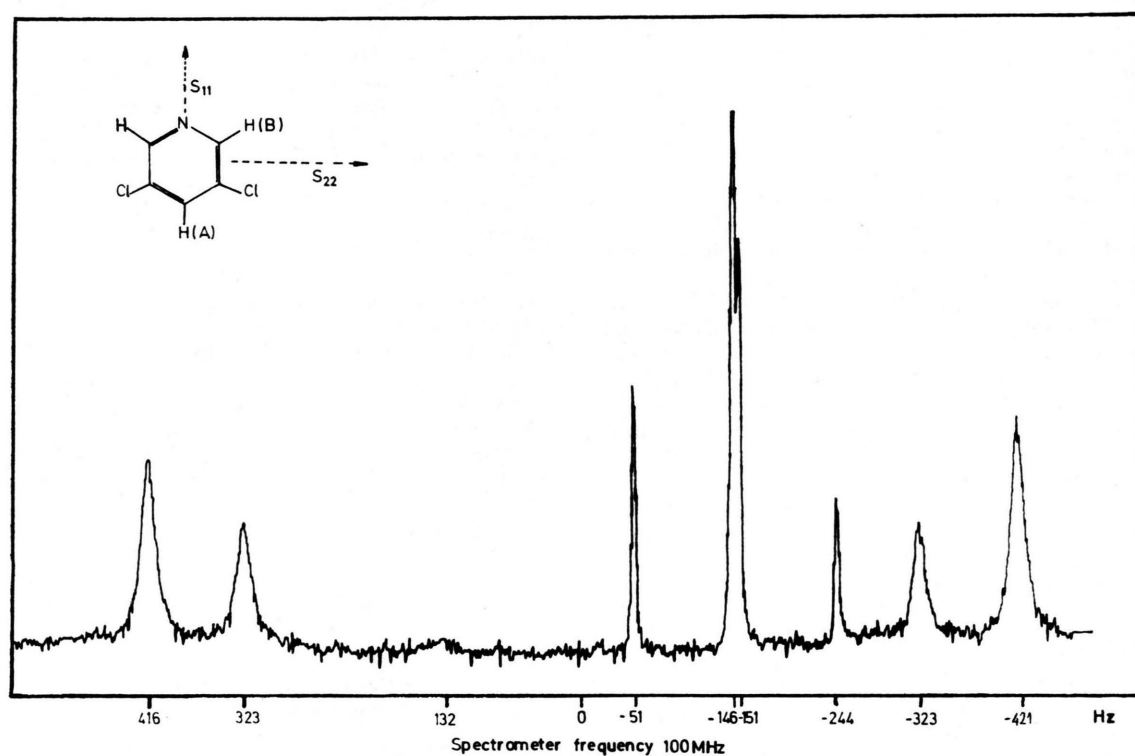


Fig. 1. The spectrum of an AB₂ symmetry with nine detected lines.

¹ P. DIEHL and C. L. KHETRAPAL, NMR Basic Principles and Progress, Vol. 1, ed. P. DIEHL, E. FLUCK, and R. KOSFELD, Springer-Verlag, Berlin 1969.

² Tables of Interatomic Distances and Configuration in Molecules and Ions, ed. L. E. SUTTON, Special Publication No. 18, Chemical Society, London.



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